3-Cyclopentylpropionic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C17H28O2/c1-4-5-10-16(13-14(2)3)19-17(18)12-11-15-8-6-7-9-15/h14-16H,4,6

InchiKey: AJIYNFIZBQJLGY-UHFFFAOYSA-N

Formula: C17H28O2

SMILES: CCC#CC(CC(C)C)OC(=O)CCC1CCCC1

Mol. weight [g/mol]: 264.40

Physical Properties

Property code	Value	Unit	Source
gf	92.81	kJ/mol	Joback Method
hf	-316.79	kJ/mol	Joback Method
hfus	32.58	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.328		Crippen Method
mcvol	238.370	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	1787.20		NIST Webbook
tb	688.05	K	Joback Method
tc	895.84	K	Joback Method
tf	440.51	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.06	J/mol×K	688.05	Joback Method
cpg	703.51	J/mol×K	722.68	Joback Method
cpg	722.76	J/mol×K	757.31	Joback Method
cpg	740.86	J/mol×K	791.94	Joback Method
cpg	757.83	J/mol×K	826.57	Joback Method
cpg	773.71	J/mol×K	861.20	Joback Method
cpg	788.53	J/mol×K	895.84	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292469&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume